

[Chem. Pharm. Bull., 33, 1488 (1985)]

Application of Principal Component Analysis to the Study of Quantitative Structure-Activity Relationships by Means of Multiple Regression Analysis. TANEKAZU KUBOTA*, JIRO HANAMURA, KENJI KANO, BUNJI UNO

Some important problems in the application of multiple regression analysis (MRA) to the study of quantitative structure-activity relationships (QSAR) are the effect of so-called collinearity among the explaining variables on MRA and the chance correlation. In order to reduce these effects on MRA we have here employed a combination of principal component analysis (PCA) and MRA. This treatment also seems to be useful for the purpose of predicting new drug structures. Actual calculation results are presented for some drug series. Finally, classification of the explaining variables was done by focusing on the factor loading values of the variables.

[Chem. Pharm. Bull., 33, 5155 (1985)]

Origin of the Negative Shift of Half-Wave Reduction Potentials of Aromatic Polynuclear *p*-Quinones with Increasing Conjugation.

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The half-wave reduction potentials ($E_{1/2}^{\text{red}}$) of aromatic polynuclear *p*-quinones are negative shifted with increasing π -electron conjugation, although the $E_{1/2}^{\text{red}}$ values of usual organic substances are positive shifted with the above structure change. The main reason for this exceptional behavior of the *p*-quinones has been discussed in detail by applying the composite system method. It was concluded that the interaction between the LUMO of *p*-quinones and the HOMO of *cis*-butadiene plays an important role, so that the LUMO of the *p*-quinones is destabilized by going to a ring expansion system, leading to the negative shift of $E_{1/2}^{\text{red}}$ value.

[Bull. Chem. Soc. Jpn., 58, 424 (1985)]

The Effects of the pH and the Temperature on the Oxidation-reduction Properties of Adriamycin Adsorbed on a Mercury Electrode Surface.

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The effects of the pH and the temperature on the redox properties of the quinone moiety in adriamycin adsorbed on a mercury electrode surface have been investigated by means of cyclic d. c. voltammetry. The quinone waves have been fundamentally interpreted in terms of a two-step one-electron surface-redox reaction, even in a neutral or an alkaline solution, where the reduced product is liable to cause the following deglycosidation reaction. The analysis of the pH dependence of the standard surface-redox potential reveals that the pKa's of the phenolic hydroxyl groups among the oxidized, semiquinone, and reduced forms are 8.53, 6.93, and 6.83, respectively. The thermodynamic constants of the semiquinone formation reaction have been also determined.